Process Modeling and Optimization of DAC Systems and Novel Sorbent Materials

Daison Yancy Caballero[1,2], Ryan Hughes[1,2], Miguel Zamarripa[1,2], Benjamin Omell[1], Michael Matuszewski[1,2], Janice Steckel[1], Timothy Fout[1]

[1]National Energy Technology Laboratory (NETL); [2]NETL Site Support Contractor

Background

Objectives:

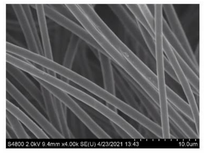
- Provide multi-scale modeling support to bench/pilot-scale tests that improve data collection and minimize uncertainty for scale-up.
- Develop contactor models of functionalized sorbent materials for direct air capture (DAC) applications.
- Leverage advanced optimization frameworks in FOQUS and/or IDAES platforms to optimize the design and operation of contactors specifically tailored to remove CO_2 from the atmosphere.

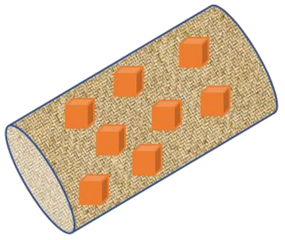
Improved Performance of Functionalized MOF Sorbent

Commercial ceramic contactors used by other DAC systems

Total CO_2 capture capacity (contactor + sorbent) (8+0)/2 = 4wt%

Amidoxime polymer adsorbent





Total CO_2 capture capacity (contactor + sorbent) (8+6)/2 = 7wt%

Contact:
Daison Caballero, NETL support contractor, Daison.YancyCaballero@netl.doe.gov
Ryan Hughes, NETL support contractor, Ryan.Hughes@netl.doe.gov

Multi-scale Modeling Framework

Development of Polymeric Sorbent Property Models

- Kinetic, equilibrium, and heat of adsorption models.
- CCSI^2 has developed tools to model isotherms from different adsorbent/metal-organic framework (MOF) materials (e.g., convex isotherms, two- and three-step isotherms).
- Pilot plant/laboratory data can be used to fit an isotherm model for the new polymeric sorbent using CCSI^2 tools.

Data Collection and Uncertainty Quantification

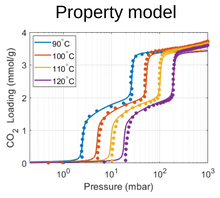
- CCSI^2 tools have been utilized for Uncertainty Quantification analysis in pilot testing campaigns to reduce uncertainty and maximize efficiency and learning from experiments.
- Uncertainty framework enables an understanding of the impacts that property data and submodels have on key process performance indicators.

Gas - Solid Contactor Models

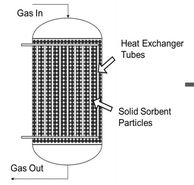
- The CCSI^2 model library includes rigorous models for fixed-bed, moving-bed, and rotary-bed reactors.
- This work will expand the model library to adapt such models for new structured materials (i.e., monolith and hollow fibers).

Model Development

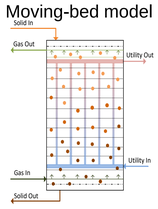
Property model



Fixed-bed model

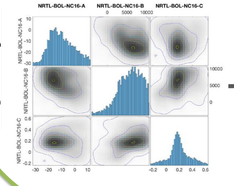


Moving-bed model

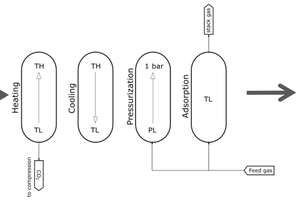


UQ Analysis

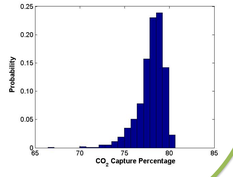
Understand uncertainty of property models/ lab scale data



Propagate uncertainty through process scale



Impacts on KPIs



Optimization Approach

- Contactor models have been developed in commercial platforms such as Aspen Adsorption and Aspen Custom Modeler that can be integrated within the CCSI Toolset for optimization and uncertainty quantification.
- Models can be implemented in the IDAES modeling platform, offering enhanced optimization capabilities (computationally faster, handles more optimization variables, etc.).

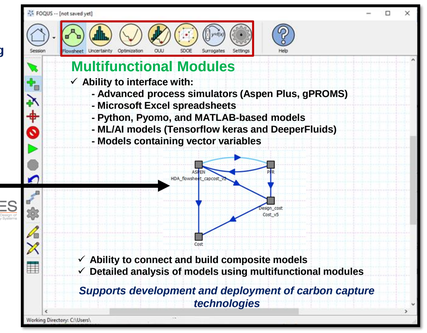
Core open-source computational tool within the CCSI-Toolset

Advanced Process Simulators and Modeling Environments

Multifunctional Modules

✓ **Ability to interface with:**
- **Advanced process simulators (Aspen Plus, gPROMS)**
- **Microsoft Excel spreadsheets**
- **Python, Pyomo, and MATLAB-based models**
- **ML/AI models (Tensorflow keras and DeeperFluids)**
- **Models containing vector variables**

PYOMO IDAES MATLAB



Comprehensive, Efficient Analysis of Process Systems

- Uncertainty Quantification.
- Simulation-Based and Hybrid Optimization.
- Surrogate Modeling (primarily ALAMO).
- Sequential Design of Experiments.
- Optimization Under Uncertainty.
- Cloud computing through AWS.

Outcome

- Develop and understand the performance of a polymeric sorbent-based, fixed-bed DAC process along with quantification of uncertainty for important model parameters.
- Guide material property development through process-scale analysis of property and hydrodynamic sub-models.
- Framework to rapidly develop updated property sub-models of new sorbent-MOF materials for optimized process performance.

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